Contents

(continued from page 4 of cover)

Role of the local electric field in electro-absorption spectra of molecular crystals
R.W. Munn 151

Interplay of creation, propagation, and relaxation of an excitation in a dimer
J. Peřina, Jr. 157

On the $O_2(v') + O_2(v'')$ atmospheric reaction. II. The role of rotational excitation
W. Wang and A.J.C. Varandas 181

The mechanism of energy transfer in H_2O–H_2O collisions – a molecular dynamics simulation
H. Svedung, L.E.B. Börjesson, N. Marković and S. Nordholm 189

Femtosecond pump–probe studies of chlorine dioxide photochemistry in water and acetonitrile
M.J. Philpott, S.C. Hayes and P.J. Reid 207

Vibrational modes in layered double hydroxides and their calcined derivatives
W. Kagunya, R. Baddour-Hadjean, F. Kooli and W. Jones 225

An intermolecular potential function for Na^+–acetonitrile obtained from ab initio calculations. Application to liquid simulations
E.M. Cabaleiro-Lago and M.A. Ríos 235

Constant temperature simulations using the Langevin equation with velocity Verlet integration
M.G. Paterlini and D.M. Ferguson 243

Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer
D. Meyer zum Büschenfelde and A. Staib 253

Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study
S. Thiel, T. Klüner and H.-J. Freund 263

Analytical theory of time-resolved fluorescence anisotropy and dynamic stokes shift of polar solute molecules based on continuum model for solvent
F. Tanaka and N. Mataga 277

Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2d_5 at low temperatures
V.L. Vyazovkin and V.A. Tolkatchev 291

Recognition and characterization of binding modes of Δ- and Λ-$[Ru(phen)_3]^{2+}$ and Δ- and Λ-$[Ru(phen)_2DPPZ]^{2+}$ by the ^{23}Na NMR relaxation and binding free energy parameters
F.C. Marincola, M. Casu, G. Saba, A. Lai, P. Lincoln and B. Nordén 301

Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S_2 state
H. Okamoto, M. Ogura, T. Nakabayashi and M. Tasumi 309

(continued on preceding page)

Contents

(continued from following page)

Emission spectra of $HeAr_2^+$ and $HeKr_2^+$ heterotrimer ions produced in a helium flowing afterglow
M. Tsuji, M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura 319

Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects
F. López Arbeloa, T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri 331

On the electronic energy disposal of calcium excited atom reactions with halogen-containing compounds: Electronic branching ratio and spin–orbit state populations
M. Garay, C.A. Rinaldi, J.M. Orea and A. González Ureña 343

Ultrafast intermolecular electron transfer in coumarin–hydrazine system
H. Shirota, H. Pal, K. Tominaga and K. Yoshihara 355

A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy
E.E. Rennie, C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova 365

Rotational alignment from the reactions $Sr(^3P_J) + CCl_4$ and $CHCl_3$
M.-L. Wang, K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He 387

Positronium formation and quenching in frozen and liquid solutions in octanol
F. Bockstahl, I. Billard, G. Duplâtre and A. Bonnenfant 393

Author index 405

Subject index 409

Instructions to authors 421